



Effective Hamiltonian models of the cross-resonance gateEaswar Magesan and Jay M. Gambetta *IBM T.J. Watson Research Center, Yorktown Heights, New York 10598, USA* (Received 29 January 2020; accepted 20 March 2020; published 5 May 2020)

Effective Hamiltonian methods are utilized to model the two-qubit cross-resonance gate for both the ideal two-qubit case and when higher levels are included. Analytic expressions are obtained in the qubit case and the higher-level model is solved both perturbatively and numerically, with the solutions agreeing well in the weak-drive limit. The methods are applied to parameters from recent experiments and, accounting for classical cross-talk effects, results in good agreement between theory and experimental results.

DOI: [10.1103/PhysRevA.101.052308](https://doi.org/10.1103/PhysRevA.101.052308)**I. INTRODUCTION**

Implementing high-fidelity quantum operations is a central problem in the field of experimental quantum information processing (QIP). Building a universal fault-tolerant quantum computer requires the ability to perform a high-fidelity two-quantum-bit (two-qubit) entangling gate and, while many proposals have been put forth for implementing two-qubit gates, few experimental demonstrations have achieved fidelities near those determined by fault-tolerant analyses [1,2]. The *cross-resonance* (CR) gate [3,4] has recently been utilized in superconducting circuit systems [5] to achieve a two-qubit CNOT gate with high fidelity exceeding 0.99 [6] and has been used in small-scale multiqubit demonstrations of fault-tolerant protocols [7–10]. Here we provide a theoretical analysis of the CR gate and outline effective Hamiltonian methods that can be used to obtain a description of the gate dynamics. The developed techniques are directly applicable in realistic systems as shown by the improved experimental calibration and high two-qubit gate fidelity of Ref. [6].

Broadly speaking, the goal of effective Hamiltonian theory is to model some set of complex dynamics on a large system via a more compact Hamiltonian on a set of smaller subsystems or subspaces. Effective Hamiltonian methods have been utilized in various areas of physics and chemistry, including nuclear, atomic-molecular, optical, and condensed-matter systems. In particular, techniques for the adiabatic elimination of higher-energy levels in a system have been widely studied, with common examples including the Schrieffer-Wolff transformation [11,12] and Born-Oppenheimer approximation [13]. Here we restrict attention to effective Hamiltonian constructions based on unitary (canonical) operations that transform the Hamiltonian H on the full Hilbert space \mathcal{H} into a block-diagonal Hamiltonian H_{eff} with the two-block case corresponding to the standard Schrieffer-Wolff transformation.

We outline the perturbative construction of an effective Hamiltonian where the desired block-diagonal form is enforced at each order. The advantage of the perturbative construction lies in obtaining analytical expressions for components of H_{eff} that hold in the weak perturbation

limit. The second construction is based on an exact multi-block-diagonalization technique [14], which finds the block-diagonal Hamiltonian that is closest to the true Hamiltonian under the principle of least action. This method has the advantage of being valid in the strong drive regime; however, it is not possible to compute general analytic expressions for the Hamiltonian components except in simple cases such as the basic two-qubit model. These methods are applied to obtain an effective model for the CR gate Hamiltonian in the two-qubit model as well as when higher levels are included. As a concrete example, we use the parameters of Ref. [6] and find good agreement between the perturbative and exact multi-block-diagonalization approaches in the weak-drive limit with higher levels included. However, a discrepancy is found between the theory and experiment since Ref. [6] finds the presence of extra unwanted terms in the Hamiltonian. We propose classical cross talk between the two transmons from the CR drive as a potential source for this discrepancy and extend the analysis to include this effect. After doing so, we find very good agreement between the theoretical predictions and experimental results of Ref. [6].

The paper is structured as follows. First, in Sec. II, we describe the starting Hamiltonian for the analysis, which consists of two transmons dispersively coupled to a resonator. We outline a method to find an effective block-diagonal Hamiltonian for the two-transmon-resonator system, which when projected onto the zero-excitation subspace of the resonator provides an effective Hamiltonian for the two-transmon system alone. Next, in Sec. III, we model the transmons as ideal qubits and find an analytic expression for the effective CR Hamiltonian under the principle of least action. In Sec. IV, we model the transmons as Duffing oscillators and find perturbative expressions that hold in the weak-drive limit. We also perform a numerical analysis of the exact block-diagonalization technique using the parameters of Ref. [6]. In Sec. V, we analyze classical cross talk occurring from the CR drive to model the results of Ref. [6]. For clarity of the presentation, the mathematical methods and details of effective Hamiltonian theory are contained in Appendix A, with the main text focused mainly on discussion of the application of the methods to the CR gate.

$$\begin{bmatrix} \frac{(J^2 - \sqrt{J^2(J^2 + \Omega^2)})(\Delta + \sqrt{2J^2 + \Delta^2 + \Omega^2 + 2\sqrt{J^2(J^2 + \Omega^2)}})}{J\Omega^2} \\ - \frac{(\Delta + \sqrt{2J^2 + \Delta^2 + \Omega^2 + 2\sqrt{J^2(J^2 + \Omega^2)}})}{\Omega} \\ \frac{(J^2 + \sqrt{J^2(J^2 + \Omega^2)})}{J\Omega} \\ 1 \end{bmatrix},$$

$$\begin{bmatrix} \frac{-(J^2 + \sqrt{J^2(J^2 + \Omega^2)})(-\Delta + \sqrt{2J^2 + \Delta^2 + \Omega^2 - 2\sqrt{J^2(J^2 + \Omega^2)}})}{J\Omega^2} \\ \frac{(-\Delta + \sqrt{2J^2 + \Delta^2 + \Omega^2 - 2\sqrt{J^2(J^2 + \Omega^2)}})}{\Omega} \\ \frac{(J^2 - \sqrt{J^2(J^2 + \Omega^2)})}{J\Omega} \\ 1 \end{bmatrix},$$

$$\begin{bmatrix} \frac{-(J^2 + \sqrt{J^2(J^2 + \Omega^2)})(-\Delta + \sqrt{2J^2 + \Delta^2 + \Omega^2 + 2\sqrt{J^2(J^2 + \Omega^2)}})}{J\Omega^2} \\ \frac{(-\Delta + \sqrt{2J^2 + \Delta^2 + \Omega^2 + 2\sqrt{J^2(J^2 + \Omega^2)}})}{\Omega} \\ \frac{(J^2 + \sqrt{J^2(J^2 + \Omega^2)})}{J\Omega} \\ 1 \end{bmatrix}.$$

Approximating

$$\frac{(J^2 \pm \sqrt{J^2(J^2 + \Omega^2)})}{J\Omega} \sim 1, \quad (3.4)$$

and rescaling the eigenvectors implies that \bar{X} takes the form

$$\begin{bmatrix} 1 \\ -1 \\ -\frac{\Omega}{(\Delta + \sqrt{J^2 + \Delta^2 + (\Omega - J)^2})} \\ \frac{\Omega}{(\Delta + \sqrt{J^2 + \Delta^2 + (\Omega - J)^2})} \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 1 \\ -\frac{\Omega}{(\Delta + \sqrt{J^2 + \Delta^2 + (\Omega + J)^2})} \\ -\frac{\Omega}{(\Delta + \sqrt{J^2 + \Delta^2 + (\Omega + J)^2})} \end{bmatrix}, \quad (3.5)$$

$$\begin{bmatrix} 1 \\ -1 \\ \frac{\Omega}{(-\Delta + \sqrt{J^2 + \Delta^2 + (\Omega - J)^2})} \\ -\frac{\Omega}{(-\Delta + \sqrt{J^2 + \Delta^2 + (\Omega - J)^2})} \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 1 \\ \frac{\Omega}{(-\Delta + \sqrt{J^2 + \Delta^2 + (\Omega + J)^2})} \\ \frac{\Omega}{(-\Delta + \sqrt{J^2 + \Delta^2 + (\Omega + J)^2})} \end{bmatrix}. \quad (3.6)$$

The least-action unitary T that block diagonalizes H_R is given by

$$T = X X_{\text{BD}}^\dagger X_P^{-\frac{1}{2}}, \quad (3.7)$$

where X_{BD} is the block diagonalization of X and $X_P = X_{\text{BD}} X_{\text{BD}}^\dagger$. We have

$$(\bar{X}_P)^{-\frac{1}{2}}(1 : 2, 1 : 2) = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}, \quad (3.8)$$

and $(\bar{X}_P)^{-\frac{1}{2}}(3 : 4, 3 : 4)$ is the 2×2 matrix

$$\begin{bmatrix} a & b \\ b & a \end{bmatrix}, \quad (3.9)$$

where

$$a = \frac{-2\Delta + \sqrt{J^2 + \Delta^2 + (\Omega - J)^2} + \sqrt{J^2 + \Delta^2 + (\Omega + J)^2}}{2\sqrt{2}\Omega},$$

$$b = \frac{-\sqrt{J^2 + \Delta^2 + (\Omega - J)^2} + \sqrt{J^2 + \Delta^2 + (\Omega + J)^2}}{2\sqrt{2}\Omega}. \quad (3.10)$$

Ignoring terms of the order of J^2 gives the following unnormalized columns for T :

$$\begin{bmatrix} \sqrt{2} \\ 0 \\ \frac{-\sqrt{2}\Omega}{(\Delta + \sqrt{\Delta^2 + \Omega^2})} \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ \sqrt{2} \\ 0 \\ \frac{-\sqrt{2}\Omega}{(\Delta + \sqrt{\Delta^2 + \Omega^2})} \end{bmatrix},$$

$$\begin{bmatrix} \sqrt{2} \\ 0 \\ \frac{-\sqrt{2}\Omega}{(\Delta - \sqrt{\Delta^2 + \Omega^2})} \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ \sqrt{2} \\ 0 \\ \frac{-\sqrt{2}\Omega}{(\Delta - \sqrt{\Delta^2 + \Omega^2})} \end{bmatrix}. \quad (3.11)$$

Finally, computing the block diagonal of H_R and moving back to the physical frame consisting of the transmons rotating at their respective frequencies gives the block-diagonal Hamiltonian H_{CR} with 2×2 blocks given by

$$\frac{1}{2} \begin{bmatrix} \Delta - \sqrt{\Delta^2 + \Omega^2} & -\frac{J\Omega}{\sqrt{\Delta^2 + \Omega^2}} \\ -\frac{J\Omega}{\sqrt{\Delta^2 + \Omega^2}} & \Delta - \sqrt{\Delta^2 + \Omega^2} \end{bmatrix}, \quad (3.12)$$

$$\frac{1}{2} \begin{bmatrix} -\Delta + \sqrt{\Delta^2 + \Omega^2} & \frac{J\Omega}{\sqrt{\Delta^2 + \Omega^2}} \\ \frac{J\Omega}{\sqrt{\Delta^2 + \Omega^2}} & -\Delta + \sqrt{\Delta^2 + \Omega^2} \end{bmatrix}. \quad (3.13)$$

The ZX term is thus given by

$$\text{tr}\left(H_{\text{CR}} \left[\frac{ZX}{2} \right] \right) = -\frac{J\Omega}{\sqrt{\Delta^2 + \Omega^2}}, \quad (3.14)$$

where, by virtue of the system Hamiltonian definition, the two-qubit Pauli operators are scaled by $\frac{1}{2}$ (in an n -qubit system, they are scaled by $\frac{1}{2^{n-1}}$). The Stark-shift term on the control qubit is given by

$$\text{tr}\left(H_{\text{CR}} \left[\frac{ZI}{2} \right] \right) = \Delta - \sqrt{\Delta^2 + \Omega^2}, \quad (3.15)$$

and so, in total,

$$H_{\text{CR}} = (\Delta - \sqrt{\Delta^2 + \Omega^2}) \frac{Z\mathbb{1}}{2} - \left(\frac{J\Omega}{\sqrt{\Delta^2 + \Omega^2}} \right) \frac{ZX}{2}. \quad (3.16)$$

IV. EFFECTIVE CR HAMILTONIAN FOR A HIGHER-LEVEL MODEL

For a model including higher levels, the approach is to first dress $H_{\text{sys}}^{(0)}$ in Eq. (2.12) and then rotate the drive term into this frame. The system is then moved into the frame rotating at the target qubit frequency on both qubits, and an RWA

is performed. In this rotating frame, the control $|0\rangle$ and $|1\rangle$ states define two subspaces that are far detuned by $\sim\Delta$ and an effective block-diagonal Hamiltonian is obtained via the perturbative analysis of Appendix A 2. Unlike the qubit case, exact analytical expressions are not straightforward to obtain and so realistic parameters are used for the exact method of Appendix A 1. For these parameters, we find that the perturbative expressions and the exact block diagonalization agree up to medium power drives of $\Omega \sim 50$ MHz, with the exact method holding for much larger values of Ω . Note that a semianalytical approach to estimating rates for the CR gate has been given in Ref. [17].

To start, we assume that $\frac{J}{|\tilde{\omega}_1 - \tilde{\omega}_2|} \ll 1$ and obtain an effective diagonal Hamiltonian for $H_{\text{sys}}^{(0)}$. Letting U be the diagonalizing (dressing) unitary, the effective diagonal Hamiltonian is given by

$$\tilde{H}_{\text{sys}}^{(0)} = U^\dagger H_{\text{sys}}^{(0)} U, \quad (4.1)$$

where, to second order in the two-qubit subspace,

$$\tilde{H}_{\text{sys}}^{(0)} = \omega_1 \frac{Z\mathbb{1}}{2} + \omega_2 \frac{\mathbb{1}Z}{2} + \xi \frac{ZZ}{2}, \quad (4.2)$$

with

$$\omega_1 = -\tilde{\omega}_1 - \frac{J^2}{\Delta} - \xi, \quad (4.3)$$

$$\omega_2 = -\tilde{\omega}_2 + \frac{J^2}{\Delta} - \xi, \quad (4.4)$$

$$\xi = -\frac{J^2(\delta_1 + \delta_2)}{(\Delta + \delta_1)(\delta_2 - \Delta)}. \quad (4.5)$$

The presence of higher levels has produced an effective ZZ interaction in the two-qubit subspace. The drive term of Eq. (2.14) is rotated into this frame by applying the diagonalizing unitary U ,

$$\tilde{H}_d = \sum_{j=1}^2 [\Omega_{X_j}(t) \cos(\omega_{d_j} t) + \Omega_{Y_j}(t) \sin(\omega_{d_j} t)] \tilde{B}_j, \quad (4.6)$$

where $\tilde{B}_j = U^\dagger (b_j^\dagger + b_j) U$ for $j = 1, 2$. We set $\omega_{d_1} = \omega_{d_2} = \omega_d$ and the Hamiltonian in the dressed frame is given by

$$H(t) = \tilde{H}_{\text{sys}}^{(0)} + \tilde{H}_d(t). \quad (4.7)$$

Moving into the frame rotating at ω_d on both transmons and making the RWA as outlined in Appendix B gives the Hamiltonian

$$H_{\text{RWA}} = \tilde{H}_{\text{drift}} + \tilde{H}_{d, \text{RWA}}, \quad (4.8)$$

where

$$\begin{aligned} \tilde{H}_{\text{drift}} &:= \tilde{H}_{\text{sys}}^{(0)} - \tilde{H}_A, \\ \tilde{H}_{d, \text{RWA}} &:= (R^\dagger \tilde{H}_d R)^{\text{RWA}}, \\ \tilde{H}_A &= \omega_d (b_1^\dagger b_1 + b_2^\dagger b_2), \end{aligned} \quad (4.9)$$

and the matrix elements of $(R^\dagger H_{d, \text{diag}} R)^{\text{RWA}}$ are given by the cases in Eq. (B1). The drive frequency on the control transmon, ω_d , is set to be the average of the dressed target transmon frequencies over the ground and excited states of

the control transmon,

$$\omega_d = \frac{\tilde{H}_{\text{sys}}^{(0)}(11) - \tilde{H}_{\text{sys}}^{(0)}(10) + \tilde{H}_{\text{sys}}^{(0)}(01) - \tilde{H}_{\text{sys}}^{(0)}(00)}{2}. \quad (4.10)$$

We suppose the states are ladder ordered as $\{00, 01, 10, 11, 02, 20, 03, 12, 21, 30, \dots, 0d, \dots, d0\}$, with F denoting the permutation matrix that moves to ladder ordering from standard Kronecker ordering. To second order in J , the $\{00, 01\}$ subspace has energy $\frac{J^2}{\Delta}$, the $\{10, 11\}$ subspace has energy $\Delta + \frac{J^2}{\Delta}$, and $\{\text{rest}\}$ is assumed to be detuned from both of these subspaces. Loosely speaking, the energy of the state $|jk\rangle$ is given by

$$j\Delta + \frac{j(j-1)}{2}\delta_1 + \frac{k(k-1)}{2}\delta_2, \quad (4.11)$$

so that H_{drift} is naturally partitioned according to the relative detunings with respect to ω_d . Therefore, the space can be partitioned as $\{00, 01\}$, $\{10, 11\}$, $\{\text{rest}\}$. The off-diagonal elements have a magnitude set by $\Omega(\frac{J}{\Delta})^m$ for $m \geq 0$. Let us now analyze the perturbative approach to obtain analytic expressions in the weak-drive limit and then investigate the exact method under the principle of least action.

A. Effective perturbative Hamiltonian

Under the assumption $\frac{\Omega}{\Delta} \ll 1$, a canonical transformation can be perturbatively constructed to find an effective block-diagonal Hamiltonian via the method outlined in Appendix A 2 b. We assume that the drive term in Eq. (4.6) contains only a drive on the X quadrature of the control with a constant amplitude Ω . The unperturbed Hamiltonian, denoted H_0 , can be defined in a few different ways. For instance, it can be defined via the block diagonals of H_{RWA} ,

$$H_0 = P_{0001} H_{\text{RWA}} P_{0001} + P_{1011} H_{\text{RWA}} P_{1011} + P_{\text{rest}} H_{\text{RWA}} P_{\text{rest}}, \quad (4.12)$$

with the perturbative term given by

$$H_1 = \frac{H_{\text{RWA}} - H_0}{\Omega}, \quad (4.13)$$

so that

$$H_{\text{RWA}} = H_0 + \lambda H_1. \quad (4.14)$$

Unfortunately, defining H_0 to be block diagonal does not provide simple analytic expressions for the effective block-diagonal Hamiltonian components because one needs to analytically compute the inverse of H_0 (see Appendix A 2 b). As a result, we approach the construction by defining an unperturbed Hamiltonian via the diagonals of H_{RWA} ,

$$H_0 = \text{diag}(H_{\text{RWA}}), \quad (4.15)$$

and define the perturbative term by

$$H_1 = \frac{H_{\text{RWA}} - H_0}{\Omega}. \quad (4.16)$$

At each order, we enforce block diagonality as usual, where the diagonal unperturbed Hamiltonian is treated as block diagonal. In this picture, all terms of the Hamiltonian containing the drive are included in the perturbation Hamiltonian and the

inverse of H_0 is simple to compute. The order parameter is given by $\lambda = \Omega$ and

$$H_{\text{RWA}} = H_0 + \lambda H_1. \quad (4.17)$$

The perturbation proceeds as follows. The effective Hamiltonian takes the form

$$H_{\text{eff}} = \sum_{m=0}^{\infty} \lambda^m H^{(m)}, \quad (4.18)$$

where $H^{(0)} = H_0$ is diagonal (block diagonal) and, for $m > 0$,

$$H^{(m)} = i[S^{(m)}, H_0] + H_x^{(m)}, \quad (4.19)$$

with $H_x^{(m)}$ defined in Appendix A 2 b. We define the m th-order approximation to H_{eff} by

$$H_{\text{eff}}^{(m)} = H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \dots + \lambda^m H^{(m)}, \quad (4.20)$$

where, at each order, $H^{(m)}$ is enforced to be block diagonal by the choice of $S^{(m)}$. Usually for $m = 1$, $H_x^{(1)} = H_1$ is orthogonal to the desired form of $H_{\text{eff}}^{(m)}$ and so $S^{(1)}$ typically eliminates the first-order term $H^{(1)}$. Here, however, by choosing H_0 to be diagonal, H_1 has nonzero super- and subdiagonals of the order of $\frac{J}{\Delta}\Omega$. Therefore, while we assume as usual that $S^{(1)}$ is off-block-diagonal, the nonzero super- and subdiagonals of H_1 survive to give a contribution at first order in Ω so that $H_{\text{eff}}^{(1)}$ has leading diagonals of the order of $\frac{J}{\Delta}\Omega$ and unchanged diagonal elements (which have shifts of the order of $\frac{J^2}{\Delta}$ from the dressing).

Keeping terms to first order in J ,

$$H_x^{(2)} = -\frac{1}{2}[S^{(1)}, [S^{(1)}, H_0]] + i[S^{(1)}, H_1] \quad (4.21)$$

has sub- and superdiagonals equal to 0 and contributions of the order of Ω^2 on the diagonals. Thus the second-order term contributes only to the diagonals, and the off diagonals of $H_{\text{eff}}^{(2)}$ are the same as in the first-order expression,

$$\begin{aligned} H_{\text{eff}}^{(1)}[1, 2] &= H_{\text{eff}}^{(2)}[1, 2] = -\frac{J\Omega_{X,1}}{2\Delta}, \\ H_{\text{eff}}^{(1)}[3, 4] &= H_{\text{eff}}^{(2)}[3, 4] = -\frac{J\Omega_{X,1}(\Delta - \delta_1)}{2\Delta(\Delta + \delta_1)}. \end{aligned} \quad (4.22)$$

Going to third order, one again obtains corrections to the off diagonals and we use the third-order effective Hamiltonian for the analytic expressions of the Hamiltonian. Moving back into the physical frame to restore the correct energies relative to the respective qubit frequencies gives the final Hamiltonian H_{CR} ,

$$H_{\text{CR}} = H_{\text{eff}} + (\omega_d - \omega_{d_1})F(b^\dagger b \otimes \mathbb{1})F^\dagger, \quad (4.23)$$

where

$$\omega_{d_1} = \frac{\tilde{H}_{\text{sys}}^{(0)}(11) - \tilde{H}_{\text{sys}}^{(0)}(01) + \tilde{H}_{\text{sys}}^{(0)}(10) - \tilde{H}_{\text{sys}}^{(0)}(00)}{2} \quad (4.24)$$

is the dressed frequency of the control qubit.

The ZX coefficient to third order is given by

$$\begin{aligned} \frac{ZX}{2} \text{coeff} &= \frac{ZX}{2} \text{linear} + \frac{J\Omega^3\delta_1^2(3\delta_1^3 + 11\delta_1^2\Delta + 15\delta_1\Delta^2 + 9\Delta^3)}{2\Delta^3(\delta_1 + \Delta)^3(\delta_1 + 2\Delta)(3\delta_1 + 2\Delta)}, \end{aligned} \quad (4.25)$$

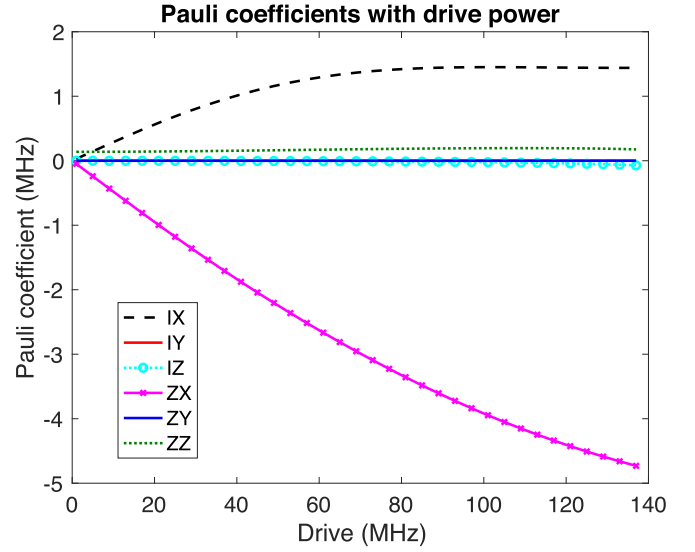


FIG. 1. All Pauli coefficients excluding ZI as a function of CR drive amplitude for model including higher levels.

where

$$\frac{ZX}{2} \text{linear} = -\frac{J\Omega}{\Delta} \left(\frac{\delta_1}{\delta_1 + \Delta} \right), \quad (4.26)$$

and the full set of Pauli coefficients is given in Appendix C. The poles in the ZX expression occur at $\Delta = 0$, $-\frac{\delta_1}{2}$, $-\delta_1$, $-\frac{3\delta_1}{2}$. The point $\Delta = 0$ corresponds to the qubits on-resonance and the point $\Delta = -\delta_1$ corresponds to the $\omega_{01}^{(1)} = \omega_{12}^{(2)}$. The points $\Delta = -\frac{\delta_1}{2}$ and $\Delta = -\delta_1, -\frac{3\delta_1}{2}$ are two-photon processes, the first of which corresponds to $\omega_{01}^{(1)} = \frac{\omega_{02}^{(2)}}{2}$. If these points are avoided, one expects the perturbative expressions to model the system well in the weak-drive limit. Low-order perturbative analysis has been utilized in Ref. [18] to better understand the operating regime.

B. Effective Hamiltonian from principle of least action

An effective block-diagonal CR Hamiltonian obtained under the principle of least action (outlined in Appendix A 1) provides a valid model in the limit of strong drives, where the perturbative model breaks down. Since a general analytic expression for the effective Hamiltonian cannot be obtained, we use the device parameters of Ref. [6] to form the basis of our study: $\omega_1/2\pi = 5.114$ GHz, $\omega_2/2\pi = 4.914$ GHz, $\delta_1/2\pi = -0.330$ GHz, $\delta_2/2\pi = -0.330$ GHz, $g_1/2\pi = 0.098$ GHz, $g_2/2\pi = 0.083$ GHz, $\omega_r/2\pi = 6.31$ GHz, and $\xi/2\pi = 277$ kHz. Using the approximation from Eq. (4.5),

$$\xi = -\frac{2J^2(\delta_1 + \delta_2)}{(\Delta_{12} + \delta_1)(\delta_2 - \Delta_{12})}, \quad (4.27)$$

the exchange coupling rate is given by $J/2\pi = 3.8$ MHz. Figure 1 contains all of the relevant Pauli coefficients except ZI, which is given in Fig. 2 and diverges quickly since the control qubit is driven far off resonance. The presence of higher levels and finite anharmonicity produces a large IX term in the Hamiltonian that is not present in the pure qubit model. The ZX and IX coefficients have the largest magnitude

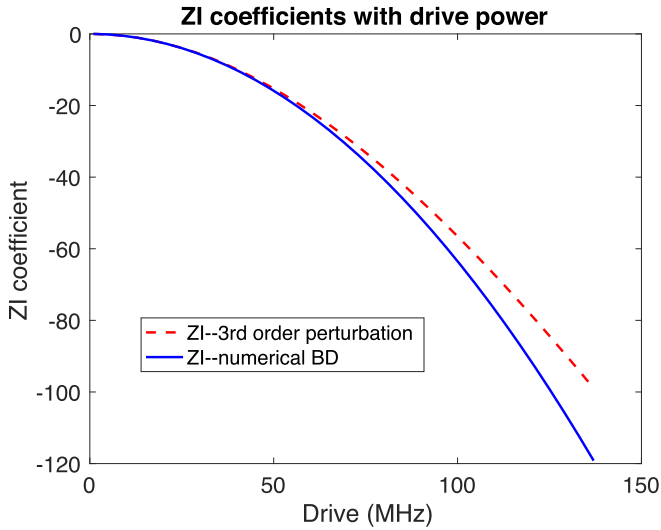


FIG. 2. ZI Pauli coefficient as a function of CR drive amplitude for model including higher levels.

and so the other coefficients are also contained alone in Fig. 3. The IZ and ZZ terms do not deviate significantly from their initial values as the drive amplitude increases. Note that the nonzero offset of the ZZ coefficient corresponds to the static ZZ term.

Importantly, there is no IY term present, which is also expected from the perturbative expressions for the Pauli coefficients in Appendix C. This is in contrast to the experimental results of Ref. [6], where there is a large IY component for this set of parameters. We revisit this discrepancy in Sec. V. Figure 4 contains expressions for the ZX term from the different Hamiltonian models: principle of least action, first-order perturbative expression, third-order perturbative expression, and the ideal qubit limit. As expected, the perturbative expressions match the principle of least action for weak Ω , but diverge as Ω grows large. In addition, there is a significant deviation between the ZX coefficient for the perfect qubit model and

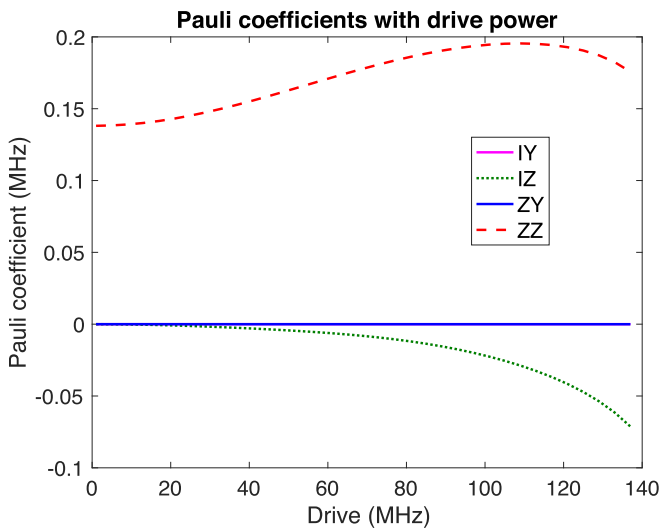


FIG. 3. IY , IZ , ZY , and ZZ Pauli coefficients as a function of CR drive amplitude for model including higher levels.

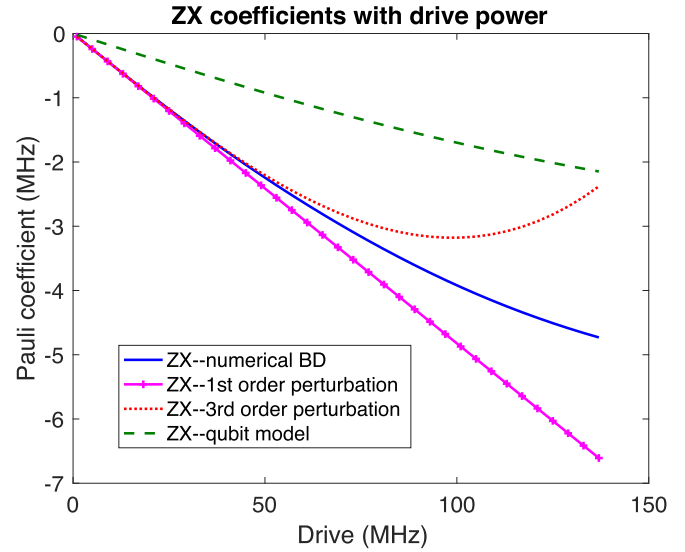


FIG. 4. Perturbative, qubit model, and numerical ZX values as a function of CR drive amplitude.

that from the principle of least action, which indicates that the presence of higher levels with finite anharmonicity needs to be taken into account for accurate Hamiltonian modeling.

Next, both the frequency of the control transmon, ω_1 , and the drive amplitude Ω are swept with $\Delta/2\pi$ varied from 0 to 600 MHz and $\Omega/2\pi$ from 0 to 100 MHz. From the poles in the expressions of the Pauli coefficients found in Sec. IV A, one expects that when $\Delta = -\frac{\delta_1}{2}, -\delta_1, -\frac{3\delta_1}{2}$, H_{eff} will be a poor model for H . A method for quantifying how well H_{eff} captures the full dynamics is discussed in Appendix A 1. The ZX coefficient is shown in Fig. 5 and, up to $-\delta_1$, there is a sizable ZX rate; however, past this point, the rate quickly goes to 0. Intuitively, this phenomenon is explained by the fact that when two transmons are detuned by an amount greater than their anharmonicity, they begin to look like harmonic oscillators

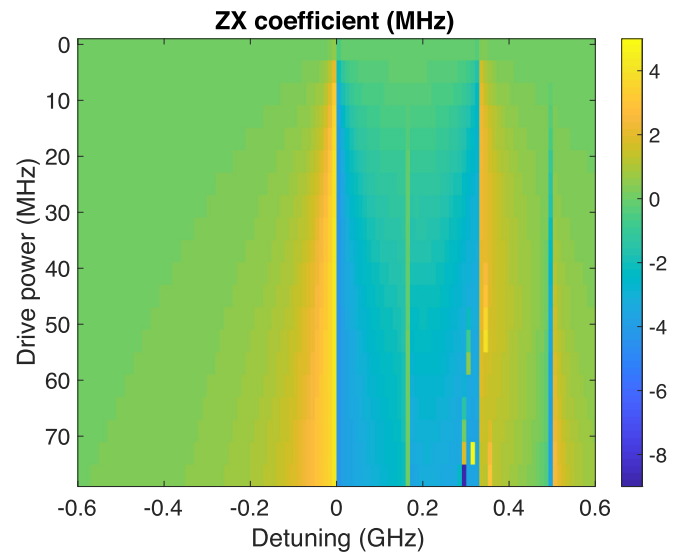


FIG. 5. Two-dimensional ZX coefficient sweep (color scale in MHz).

with respect to each other. Therefore, since entanglement cannot be created between two harmonic oscillators, the ZX term approaches 0 as the detuning Δ grows large.

V. MODELING CLASSICAL CROSS TALK FROM CR DRIVE

In Ref. [6], a CR gate with the parameters of Sec. IV B was calibrated based on the block-diagonal effective Hamiltonian in a scheme called partial Hamiltonian tomography. A large IY term was found to be present, but clearly the results of Sec. IV B predict no such term can arise from the Hamiltonian model considered to this point. One potential model for the source of this term that we investigate here is *classical cross talk* induced on the target from driving the control.

To analyze this model, we go back to Eq. (4.6) and allow for a drive term on the target qubit whose amplitude and phase depend on the drive on the control. The total drive term then takes the form

$$\tilde{H}_d = \Omega(t) \cos(\omega_d t + \phi_c) \tilde{B}_1 + A \Omega(t) \cos(\omega_d t + \phi_t) \tilde{B}_2, \quad (5.1)$$

where $\tilde{B}_j = U^\dagger (b_j^\dagger + b_j) U$ for $j = 1, 2$, $A \leq 1$ is a scale factor modeling the amplitude of the cross-talk term, and ϕ_t is the phase lag that occurs on the target. The values of these parameters depend on the form of the cross-talk channel. Since the cross-talk term corresponds directly to a rotation on the target qubit, the condition for block diagonalization $\frac{\Omega}{\Delta_{12}} \ll 1$ is unchanged and the methods discussed here can be used to obtain an effective Hamiltonian.

Using the parameters of Ref. [6], we find the following values for A , ϕ_c , and ϕ_t :

$$A = 0.071, \quad \phi_c = \pi, \quad \phi_t = -0.62, \quad (5.2)$$

produce the Pauli coefficients seen in Fig. 6, which agree well with those in Fig. 2(b) of Ref. [6]. It is important to note that this agreement only suggests classical cross talk as a potential source for the presence of the IY term in Ref. [6]. Potential sources of cross-talk channels are an area of current investigation.

VI. DISCUSSION

We have provided detailed theoretical models of the cross-resonance gate via effective block-diagonal Hamiltonian techniques. For the idealized qubit model, analytic expressions for the Hamiltonian components using the principle of least action [14] were obtained. The only two nonzero components are a large Stark-shift term on the control qubit from off-resonant driving as well as the ZX term required for generating entanglement. For the realistic transmon model, effective Hamiltonians were constructed via both a perturbative approach as well as the principle of least action. These two approaches agree well in the weak-drive limit and predict nonzero Pauli coefficients of the form $A \otimes B$ with $A \in \{I, Z\}$, $B \in \{I, X, Z\}$. The presence of extra Hamiltonian terms compared to those from the ideal qubit case implies that higher

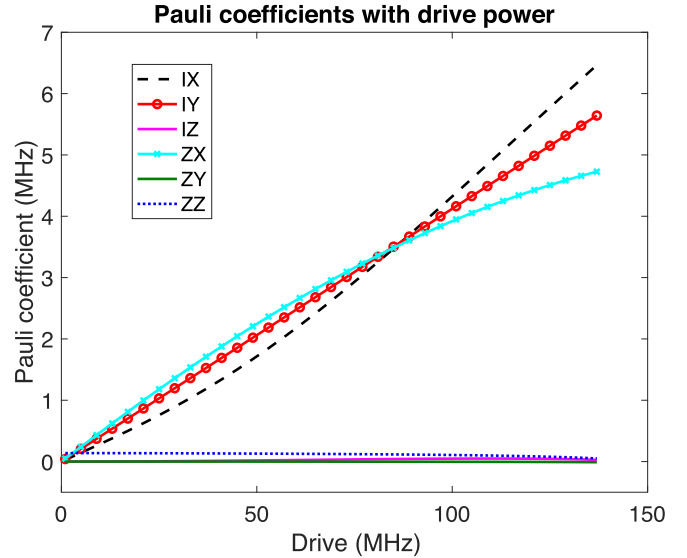


FIG. 6. All Pauli coefficients excluding ZI as a function of CR drive amplitude for model with higher levels and a drive on target representing classical cross talk.

levels play an important role to understand the precise error terms for implementing a two-qubit gate.

In the experiment of Ref. [6], an IY term was found to be present, in contrast to what is predicted from our analysis with a single CR drive on the control transmon. We propose that this discrepancy is a result of classical cross talk between the two transmons and generalized the model to include this effect via an additional phase-shifted drive term on the target transmon. For a set of realistic model parameters, we found good agreement between the theoretical results here and those of Ref. [6], which implies classical cross talk may be a significant issue in real systems. Understanding the cross-talk channels leading to drive terms on the target transmon is an important area of further research.

Various interesting questions remain as directions for future research. First, it is useful to understand whether the perturbative construction converges to that of the principle of least action. For the standard two-block Schrieffer-Wolff transformation, the perturbative construction does converge to exact unitary rotation and ideally this property holds for the multiblock case as well. It will also be interesting to apply these methods to larger multiqubit systems, especially in the context of finding points to avoid in frequency space when dealing with fixed-frequency transmons in a circuit-QED architecture. The results from a multiqubit analysis will have an impact on future design considerations in superconducting circuit systems.

ACKNOWLEDGMENTS

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APPENDIX A: EFFECTIVE HAMILTONIANS

1. Effective Hamiltonian from principle of least action

Suppose one is given a Hamiltonian H on the Hilbert space \mathcal{H} with eigenvalues E_a and eigenvectors $|s_a\rangle$,

$$H = \sum_a E_a |s_a\rangle\langle s_a|.$$

A Hermitian matrix H_{eff} is said to be an effective Hamiltonian for H with respect to the orthogonal subspaces $\{\mathcal{K}_a\}$ ($\cup_a \mathcal{K}_a = \mathcal{H}$) if the following are satisfied:

- (1) H_{eff} has the same energy spectrum as H ,
- (2) H_{eff} only has support on the \mathcal{K}_a .

Suppose each subspace \mathcal{K}_a has dimension $d_{\mathcal{K}_a}$ and let $P_{\mathcal{K}_a}$ be the projector onto \mathcal{K}_a . We set an orthonormal basis for each \mathcal{K}_a , denoted $\{|q_b^{\mathcal{K}_a}\rangle\}$, $b = 1, \dots, d_{\mathcal{K}_a}$, to be the standard basis for working in coordinates. Note that for each \mathcal{K}_a , any linear combination of the $|q_b^{\mathcal{K}_a}\rangle$ is still supported only on \mathcal{K}_a . The full orthonormal basis for \mathcal{H} comprised of the union of these bases will be denoted $\{|q_a\rangle\}$. H_{eff} is uniquely defined by a unitary matrix T that maps the eigenvectors of H , $|s_a\rangle$, to the eigenvectors $|r_a\rangle$ of H_{eff} , with the eigenvalues being preserved since T is unitary. From the desired form of H_{eff} having support only on the \mathcal{K}_a , the sole restriction on the $|r_a\rangle$ is that the first $d_{\mathcal{K}_1}$ vectors have support only on \mathcal{K}_1 , the next $d_{\mathcal{K}_2}$ have support only on \mathcal{K}_2 , and so on.

Let us now discuss how to actually compute T . The first step is to map the eigenvalues of H onto the $\{|q_j\rangle\}$ basis via the eigenvector matrix X of H so that all of the freedom in computing T comes from choosing a block-diagonal (with respect to $\{|q_j\rangle\}$) unitary matrix F . Since $H = \sum_a E_a |s_a\rangle\langle s_a|$, the columns of X are equal to $|s_j\rangle$ when written with respect to the basis $\{|q_k\rangle\}$,

$$X = \sum_j |s_j\rangle\langle q_j|, \quad (\text{A1})$$

and so

$$\begin{aligned} X^\dagger H X &= \left(\sum_j |q_j\rangle\langle s_j| \right) \left(\sum_a E_a |s_a\rangle\langle s_a| \right) \left(\sum_k |s_k\rangle\langle q_k| \right) \\ &= \sum_a E_a |q_a\rangle\langle q_a|. \end{aligned}$$

The unitary matrix F now rotates into the desired eigenbasis $\{|r_j\rangle\}$ and since the $|r_j\rangle$ only have support on the subspaces \mathcal{K}_a , F represented in $|q_j\rangle$ is a unitary block-diagonal matrix. The total block-diagonalizing unitary T can be written as the composition of F with X , where X is given in Eq. (A1) and

$$F = \sum_j |r_j\rangle\langle q_j|. \quad (\text{A2})$$

It is clear the freedom in choosing H_{eff} comes entirely from choosing F . Ideally, one would like to obtain a unique H_{eff} , given H . The approach given in Ref. [14] is to solve the following optimization problem:

$$\text{argmin}_F (\|T - \mathcal{I}\|_2), \quad (\text{A3})$$

which means to find the unitary matrix F that minimizes the 2-norm (Euclidean) distance between T and \mathcal{I} . The unique

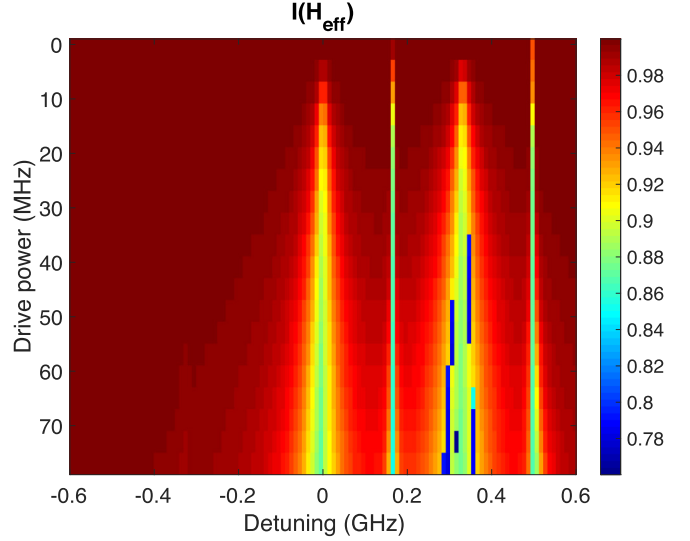


FIG. 7. $I(H_{\text{eff}})$ parameter as a function of transmon detuning and drive power.

solution of this problem is given by

$$F = \frac{X_{\text{BD}}}{\sqrt{X_{\text{BD}} X_{\text{BD}}^\dagger}},$$

where X_{BD} is the projection of X onto the subspaces \mathcal{K}_a and is assumed to be nonsingular. Intuitively, this can be thought of as first rotating H into its eigenvalue matrix and attempting to rotate back to H under the constraint of block diagonality.

There are a variety of different metrics one could use to quantify the extent to which H_{eff} captures the dynamics of H . For instance, one could directly compute the objective function in Eq. (A3). Alternatively, one can see that $H = H_{\text{eff}}$ if and only if $X = X_{\text{BD}}$ and, if the eigenvectors of H are highly mixed across different blocks, then the quality of H_{eff} as a model of H decreases. As a result, one can define a simple figure of merit, denoted $I(H_{\text{eff}})$, to be the normalized sum of the squared magnitudes of the eigenvectors of H after being projected onto the subspaces \mathcal{K}_a ,

$$I(H_{\text{eff}}) = \frac{\text{tr}(X_{\text{BD}} X_{\text{BD}}^\dagger)}{\dim(\mathcal{H})} = \frac{\|X_{\text{BD}}\|_2^2}{\dim(\mathcal{H})}.$$

Since

$$0 \leq \text{tr}(X_{\text{BD}} X_{\text{BD}}^\dagger) \leq \dim(\mathcal{H}),$$

$I(H_{\text{eff}}) \in [0, 1]$. A plot of $I(H_{\text{eff}})$ for the parameters of Ref. [6] is contained in Fig. 7, where the control transmon frequency is fixed, $\omega_1/2\pi = 5.114$ GHz. As expected, $I(H_{\text{eff}})$ deviates from 1 near the poles predicted from the perturbative analysis in Sec. IV A.

2. Effective Hamiltonian from perturbative construction of canonical transformations

In this section, we will discuss how to perturbatively obtain a canonical transformation $U = e^{-iS}$ and an effective Hamiltonian H_{eff} that describes the dynamics of our system. We will focus our attention on the case where we have an

unperturbed Hamiltonian H_0 that we can solve exactly and a perturbative term H_1 with order parameter λ , such that

$$H = H_0 + \lambda H_1.$$

Obtaining H_{eff} from H depends on the desired form we would like H_{eff} to have. Here, we derive an iterative procedure to build the Hermitian matrix S which provides the desired form of the Hamiltonian. Common examples of this method correspond to diagonalization of H and modeling the dynamics on the low-energy subspace as in the standard Schrieffer-Wolff (SW) transformation. We apply these methods to provide a complete perturbative solution to the *simultaneous block diagonalization* of H into an arbitrary number of blocks. In the case of two blocks, the standard SW transformation is recovered.

The Hermitian operator S in $U = e^{-iS}$ can be expanded as

$$S = \sum_{n=1}^{\infty} \lambda^n S_n.$$

Computing powers of S results in the expressions

$$\begin{aligned} S &= \lambda S_1 + \lambda^2 S_2 + \lambda^3 S_3 + \lambda^4 S_4 + \dots, \\ S^2 &= \lambda^2 S_1^2 + \lambda^3 (S_1 S_2 + S_2 S_1) + \lambda^4 (S_2^2 + S_1 S_3 + S_3 S_1) + \dots, \\ S^3 &= \lambda^3 S_1^3 + \lambda^4 (S_1^2 S_2 + S_1 S_2 S_1 + S_2 S_1^2) + \dots, \\ S^4 &= \lambda^4 S_1^4 + \dots. \end{aligned}$$

We can expand $U = e^{\pm iS}$ in an exponential series to obtain

$$\begin{aligned} e^{\pm iS} &= \mathbb{1} \pm i(\lambda S_1 + \lambda^2 S_2 + \lambda^3 S_3 + \lambda^4 S_4 + \dots) \\ &\quad - \frac{1}{2!} [\lambda^2 S_1^2 + \lambda^3 (S_1 S_2 + S_2 S_1 + \dots) \\ &\quad + \lambda^4 (S_2^2 + S_1 S_3 + S_3 S_1 + \dots)] \\ &\quad \mp \frac{i}{3!} [\lambda^3 S_1^3 + \lambda^4 (S_1^2 S_2 + S_1 S_2 S_1 + S_2 S_1^2) + \dots] \\ &\quad + \frac{1}{4!} (\lambda^4 S_1^4 + \dots) + \dots. \end{aligned}$$

Collecting in powers of λ , we have

$$\begin{aligned} e^{\pm iS} &= \mathbb{1} + \lambda(\pm i S_1) + \lambda^2 \left(\pm i S_2 - \frac{1}{2} S_1^2 \right) \\ &\quad + \lambda^3 \left[\pm i S_3 - \frac{1}{2} (S_1 S_2 + S_2 S_1) \mp \frac{i}{6} S_1^3 \right] \\ &\quad + \lambda^4 \left[\pm i S_4 - \frac{1}{2} (S_2^2 + S_1 S_3 + S_3 S_1) \right. \\ &\quad \left. \mp \frac{i}{6} (S_1^2 S_2 + S_1 S_2 S_1 + S_2 S_1^2) + \frac{1}{24} S_1^4 \right]. \quad (\text{A4}) \end{aligned}$$

Writing

$$e^{iS} (H_0 + \lambda V) e^{-iS} = e^{iS} H_0 e^{-iS} + \lambda e^{iS} V e^{-iS},$$

we first deal with $e^{iS} H_0 e^{-iS}$, from which an expression for $\lambda e^{iS} V e^{-iS}$ will follow in a straightforward manner.

Expanding the exponentials in Eq. (A4) and collecting powers in λ gives the following coefficients at each order:

$$\begin{aligned} \underline{\lambda^0}: & H_0, \\ \underline{\lambda^1}: & i[S_1, H_0], \\ \underline{\lambda^2}: & -\frac{1}{2}[S_1, [S_1, H_0]] = -\frac{S_1^2}{2} H_0 - H_0 \frac{S_1^2}{2} + S_1 H_0 S_1, \end{aligned}$$

$$i[S_2, H_0] = iS_2 H_0 - iH_0 S_2,$$

$$\underline{\lambda^3}: i[S_3, H_0],$$

$$\begin{aligned} & -\frac{i}{6}[S_1, [S_1, [S_1, H_0]]] \\ & = i \left(\frac{3S_1^2 H_0 S_1}{6} - \frac{3S_1 H_0 S_1^2}{6} + \frac{H_0 S_1^3}{6} - \frac{S_1^3 H_0}{6} \right), \end{aligned}$$

and

$$\begin{aligned} & -\frac{1}{2}([S_1, [S_2, H_0]] + [S_2, [S_1, H_0]]) \\ & = \frac{1}{2}(2S_1 H_0 S_2 + 2S_2 H_0 S_1 - H_0 S_1 S_2 \\ & \quad - H_0 S_2 S_1 - S_1 S_2 H_0 - S_2 S_1 H_0), \end{aligned}$$

$$\underline{\lambda^4}: i[S_4, H_0],$$

$$\begin{aligned} & -\frac{i}{6}([S_1, [S_1, [S_2, H_0]]] + [S_1, [S_2, [S_1, H_0]]] \\ & \quad + [S_2, [S_1, [S_1, H_0]]]) \\ & = \frac{i}{6} H_0 (S_1^2 S_2 + S_1 S_2 S_1 + S_2 S_1^2) \\ & \quad + -\frac{i}{6} (S_1^2 S_2 + S_1 S_2 S_1 + S_2 S_1^2) H_0 \\ & \quad - \frac{i}{2} S_1 H_0 (S_1 S_2 + S_2 S_1) - \frac{i}{2} S_2 H_0 S_1^2 \\ & \quad + \frac{i}{2} S_1^2 H_0 S_2 + \frac{i}{2} (S_1 S_2 + S_2 S_1) H_0 S_1, \end{aligned}$$

$$\begin{aligned} & \frac{1}{24}[S_1, [S_1, [S_1, [S_1, H_0]]]] \\ & = \frac{1}{24}(H_0 S_1^4 - 4S_1 H_0 S_1^3 + 6S_1^2 H_0 S_2^2 - 4S_1^3 H_0 S_2 + S_1^4 H_0), \\ & -\frac{1}{2}[S_2, [S_2, H_0]] \\ & = -\frac{1}{2}(H_0 S_2^2 - 2S_2 H_0 S_2 + S_2^2 H_0), \\ & -\frac{1}{2}([S_1, [S_3, H_0]] + [S_3, [S_1, H_0]]) \\ & = -\frac{1}{2}[H_0 (S_1 S_3 + S_3 S_1) - 2S_1 H_0 S_3 - 2S_3 H_0 S_1 \\ & \quad + (S_1 S_3 + S_3 S_1) H_0]. \end{aligned}$$

This gives, to fifth order in λ ,

$$\begin{aligned} e^{iS} H_0 e^{-iS} &= H_0 + \lambda(i[S_1, H_0]) \\ & \quad + \lambda^2 \left(i[S_2, H_0] - \frac{1}{2}[S_1, [S_1, H_0]] \right) \\ & \quad + \lambda^3 \left\{ i[S_3, H_0] - \frac{i}{6}[S_1, [S_1, [S_1, H_0]]] \right. \end{aligned}$$

$$\begin{aligned}
& -\frac{1}{2}([S_1, [S_2, H_0]] + [S_2, [S_1, H_0]]) \Big\} \\
& + \lambda^4 \left\{ i[S_4, H_0] - \frac{i}{6}([S_1, [S_1, [S_2, H_0]]) \right. \\
& \times [S_1, [S_2, [S_1, H_0]]] + [S_2, [S_1, [S_1, H_0]]) \\
& + \frac{1}{24}[S_1, [S_1, [S_1, [S_1, H_0]]]] - \frac{1}{2}[S_2, [S_2, H_0]] \\
& \left. - \frac{1}{2}([S_1, [S_3, H_0]] + [S_3, [S_1, H_0]]) \right\}.
\end{aligned}$$

Replacing H_0 with λV , we see that to fifth order in λ ,

$$\begin{aligned}
e^{iS} \lambda V e^{-iS} &= \lambda V + \lambda^2 (i[S_1, V]) \\
& + \lambda^3 \left(i[S_2, V] - \frac{1}{2}[S_1, [S_1, V]] \right) \\
& + \lambda^4 \left\{ i[S_3, V] - \frac{i}{6}[S_1, [S_1, [S_1, V]]] \right. \\
& \left. - \frac{1}{2}([S_1, [S_2, V]] + [S_2, [S_1, V]]) \right\}.
\end{aligned}$$

Hence, in total,

$$\begin{aligned}
e^{iS} (H_0 + \lambda V) e^{-iS} &= H_0 + \lambda (i[S_1, H_0] + V) \\
& + \lambda^2 \left(i[S_2, H_0] - \frac{1}{2}[S_1, [S_1, H_0]] + i[S_1, V] \right) \\
& + \lambda^3 \left\{ i[S_3, H_0] - \frac{i}{6}[S_1, [S_1, [S_1, H_0]]] \right. \\
& - \frac{1}{2}([S_1, [S_2, H_0]] + [S_2, [S_1, H_0]]) \\
& + i[S_2, V] - \frac{1}{2}[S_1, [S_1, V]] \Big\} + \lambda^4 \left\{ i[S_4, H_0] \right. \\
& - \frac{i}{6}([S_1, [S_1, [S_2, H_0]]] + [S_1, [S_2, [S_1, H_0]]) \\
& + [S_2, [S_1, [S_1, H_0]]) + \frac{1}{24}[S_1, [S_1, [S_1, [S_1, H_0]]]] \\
& - \frac{1}{2}[S_2, [S_2, H_0]] - \frac{1}{2}([S_1, [S_3, H_0]] + [S_3, [S_1, H_0]]) \\
& + i[S_3, V] - \frac{i}{6}[S_1, [S_1, [S_1, V]]) \\
& \left. - \frac{1}{2}([S_1, [S_2, V]] + [S_2, [S_1, V]]) \right\} + O(\lambda^5). \quad (\text{A5})
\end{aligned}$$

Equation (A5) can be written in a more compact fashion by defining two sequences of functions $\{f_j = f_j(\{A_i\}_{i=1}^{j+1})\}_{j=0}^{\infty}$ and $\{H^{(j)} = H^{(j)}(\{A_i\}_{i=1}^{j+2})\}_{j=0}^{\infty}$, where the A_i are indeterminate variables indicating the number of inputs to each function,

$$\begin{aligned}
e^{iS} (H_0 + \lambda V) e^{-iS} &= \sum_{k=0}^{\infty} \lambda^k H^{(k)}(\{S_j\}_{j=1}^k, H_0, V) \\
&= \lambda^0 [f_0(H_0)]
\end{aligned}$$

$$\begin{aligned}
& + \lambda^1 [f_1(\{S_j\}_{j=1}^1, H_0) + f_0(V)] \\
& + \lambda^2 [f_2(\{S_j\}_{j=1}^2, H_0) + f_1(\{S_j\}_{j=1}^1, V)] \\
& + \lambda^3 [f_3(\{S_j\}_{j=1}^3, H_0) + f_2(\{S_j\}_{j=1}^2, V)] \\
& + \lambda^4 [f_4(\{S_j\}_{j=1}^4, H_0) + f_3(\{S_j\}_{j=1}^3, V)] \\
& + O(\lambda^5).
\end{aligned}$$

The f_j can be constructed in a straightforward manner which allows for the computation of the perturbation to any order. First, write all decompositions of $k > 0$ into a sum of non-negative integers as follows:

$$\begin{aligned}
k &: (k), \\
k-1 &: (k-1, 1), (1, k-1), \\
k-2 &: (k-2, 1, 1), (1, k-2, 1), (1, 1, k-2), \\
& \quad (k-2, 2), (2, k-2), \\
k-3 &: (k-3, 1, 1, 1), (1, k-3, 1, 1), (1, 1, k-3, 1), \\
& \quad (1, 1, 1, k-3), (k-3, 1, 2), (k-3, 2, 1), \\
& \quad (1, k-3, 2), (2, k-3, 1), (1, 2, k-3), (2, 1, k-3), \\
& \quad \cdot \\
& \quad \cdot \\
& \quad \cdot \\
0 &: (1, 1, 1, \dots, 1),
\end{aligned}$$

where $(1, 1, 1, \dots, 1)$ has k indices. We now take each (j_1, \dots, j_b) from the above expression and make the assignment

$$(j_1, \dots, j_b) \rightarrow \frac{i^b}{b!} [S_{j_1}, [S_{j_2}, \dots, [S_{j_{b-1}}, [S_{j_b}, H_0]] \dots]].$$

As an example, we compute the fifth-order expression. We have

$$\begin{aligned}
& (5), \\
& (4, 1), (1, 4), \\
& (3, 1, 1), (1, 3, 1), (1, 1, 3), \\
& (3, 2), (2, 3), \\
& (2, 1, 1, 1), (1, 2, 1, 1), (1, 1, 2, 1), (1, 1, 1, 2), \\
& (2, 2, 1), (2, 1, 2), (1, 2, 2), \\
& (1, 1, 1, 1, 1).
\end{aligned}$$

This gives

$$\begin{aligned}
f_5(\{S_j\}_{j=1}^5, H_0) &= \frac{i}{1!} [S_5, H_0] - \frac{1}{2!} ([S_4, [S_1, H_0]] + [S_1, [S_4, H_0]]) \\
& - \frac{i}{3!} ([S_3, [S_1, [S_1, H_0]]] + [S_1, [S_3, [S_1, H_0]]) \\
& + [S_1, [S_1, [S_3, H_0]]] + [S_3, [S_2, H_0]] + [S_2, [S_3, H_0]]) \\
& + \frac{1}{4!} ([S_2, [S_1, [S_1, [S_1, H_0]]]] + [S_1, [S_2, [S_1, [S_1, H_0]]]]) \\
& + [S_1, [S_1, [S_2, [S_1, H_0]]]] + [S_1, [S_1, [S_1, [S_2, H_0]]]]
\end{aligned}$$

$$\begin{aligned}
& +[S_2, [S_2, [S_1, H_0]]] + [S_2, [S_1, [S_2, H_0]]] \\
& +[S_1, [S_2, [S_2, H_0]]] \\
& + \frac{i}{5!} [S_1, [S_1, [S_1, [S_1, [S_1, H_0]]]]].
\end{aligned}$$

Combining this with the expression for $f_4(\{S_j\}_{j=1}^4, V)$ already computed gives the full fifth-order term,

$$\begin{aligned}
& \lambda^5 \left[\frac{i}{1!} [S_5, H_0] - \frac{1}{2!} ([S_4, [S_1, H_0]] + [S_1, [S_4, H_0]]) \right. \\
& - \frac{i}{3!} ([S_3, [S_1, [S_1, H_0]]] + [S_1, [S_3, [S_1, H_0]]] \\
& + [S_1, [S_1, [S_3, H_0]]) + [S_3, [S_2, H_0]] + [S_2, [S_3, H_0]]) \\
& + \frac{1}{4!} ([S_2, [S_1, [S_1, [S_1, H_0]]]] + [S_1, [S_2, [S_1, [S_1, H_0]]]] \\
& + [S_1, [S_1, [S_2, [S_1, H_0]]]] + [S_1, [S_1, [S_1, [S_2, H_0]]]]) \\
& + [S_2, [S_2, [S_1, H_0]]] + [S_2, [S_1, [S_2, H_0]]] \\
& + [S_1, [S_2, [S_2, H_0]])] + \frac{i}{5!} [S_1, [S_1, [S_1, [S_1, [S_1, H_0]]]] \\
& + \left\{ i[S_4, V] - \frac{i}{6} ([S_1, [S_1, [S_2, V]]] + [S_1, [S_2, [S_1, V]]) \right. \\
& + [S_2, [S_1, [S_1, V]]) + \frac{1}{24} [S_1, [S_1, [S_1, [S_1, V]]]] \\
& \left. - \frac{1}{2} [S_2, [S_2, V]] - \frac{1}{2} ([S_1, [S_3, V]] + [S_3, [S_1, V]]) \right\} \Big].
\end{aligned}$$

Now that we can compute each f_j , we are able to recursively compute every order $H^{(j)}$. What remains is to compute the S_j , which is done by noting that at each order, $H^{(k)}(\{S_j\}_{j=1}^k, H_0, V)$ contains only one term with S_k in it, $i[S_k, H_0]$. Hence, one can write

$$\begin{aligned}
& H^{(m)}(\{S_j\}_{j=1}^m, H_0, V) \\
& = i[S_m, H_0] + H_x^{(m)}(\{S_j\}_{j=1}^{m-1}, H_0, V), \quad (\text{A6})
\end{aligned}$$

and, assuming $\{S_j\}_{j=1}^{k-1}$ have already been computed, $H_x^{(k)}$ can be computed as well. Hence, one need only solve for S_k at each order to compute $H^{(k)}$. S_k is computed by ensuring $H^{(k)}$ satisfies the required form set by the problem. We now illustrate the method with two examples: diagonalization and block diagonalization.

a. Example 1: Diagonalization

Suppose we want our effective dynamics to be diagonal at each order m , that is, we want $H^{(m)}$ to be diagonal for every m (H_0 is diagonal and V is a perturbation containing off-diagonal components). We have

$$\begin{aligned}
H^{(0)} &= H_0, \\
H_x^{(1)} &= H_1.
\end{aligned}$$

One can see from Eq. (A6) that if $H^{(m)}$ is diagonal,

$$\sum_p E_p^{(m)} |p\rangle \langle p| = i \sum_p E_p^{(0)} (S^{(m)} |p\rangle \langle p| - |p\rangle \langle p| S^{(m)}) + H_x^{(m)}. \quad (\text{A7})$$

Without loss of generality, we can assume that S is an off-diagonal matrix (has diagonal entries of 0) and so the above is satisfied if

$$\begin{aligned}
E_p^{(m)} &= \langle p | H_x^{(m)} | p \rangle, \\
\langle p | S^{(m)} | q \rangle &= \frac{-i \langle p | H_x^{(m)} | q \rangle}{E_p^{(0)} - E_q^{(0)}}, \quad p \neq q.
\end{aligned}$$

b. Example 2: Block diagonalization

Suppose we want our effective dynamics to be block diagonal at each order m , that is, we want $H^{(m)}$ to be block diagonal for every m (H_0 is block diagonal and V is a perturbation containing off-block-diagonal components). We have

$$\begin{aligned}
H^{(0)} &= H_0, \\
H_x^{(1)} &= H_1.
\end{aligned}$$

One can see from Eq. (A6) that if $H^{(m)}$ is block diagonal,

$$H^{(m)} = H_1^{(m)} \oplus \dots \oplus H_k^{(m)} \oplus \dots,$$

then acting subspace projectors P_j and P_k on both sides of Eq. (A6) give

$$\begin{aligned}
& P_j H_1^{(m)} \oplus \dots \oplus H_k^{(m)} \oplus \dots P_k \\
& = i [P_j S^{(m)} (H_1^{(0)} \oplus \dots \oplus H_k^{(0)} \oplus \dots) P_k \\
& - P_j (H_1^{(0)} \oplus \dots \oplus H_k^{(0)} \oplus \dots) S^{(m)}] P_k + P_j H_x^{(m)} P_k,
\end{aligned}$$

$$H_j^{(m)} \delta_{j,k} = i (P_j S^{(m)} P_k H_k^{(0)} - H_j^{(0)} P_j S^{(m)} P_k) + H_{x_{j,k}}^{(m)},$$

and

$$i H_{x_{j,k}}^{(m)} + H_j^{(m)} \delta_{j,k} = S_{j,k}^{(m)} H_k^{(0)} - H_j^{(0)} S_{j,k}^{(m)}.$$

Since S is an off-block-diagonal matrix (has block-diagonal entries of 0), we have

$$\begin{aligned}
H_j^{(m)} &= H_{x_{j,j}}^{(m)} \quad \text{if } j = k, \\
H_j^{(0)} S_{j,k}^{(m)} - S_{j,k}^{(m)} H_k^{(0)} &= -i H_{x_{j,k}}^{(m)} \quad \text{if } j \neq k.
\end{aligned}$$

In the case that $H^{(0)}$ is diagonal, we can solve easily for $S^{(m)}$ at each order,

$$\langle p | S_{j,k}^{(m)} | q \rangle = \frac{-i \langle p | H_{x_{j,k}}^{(m)} | q \rangle}{\langle p | H_j^{(0)} | p \rangle - \langle q | H_k^{(0)} | q \rangle}.$$

However, if $H^{(0)}$ is not diagonal, we need to use the following matrix-vector correspondence: For any A, B, C ,

$$(A \otimes B) \text{vec}(C) = \text{vec}(ACB^T),$$

where “vec” is defined as $\text{vec}(|a\rangle \langle b|) = |a\rangle \otimes |b\rangle$. Hence,

$$\begin{aligned}
AB - BC &= D \Leftrightarrow \\
AB \mathbb{1}^T - \mathbb{1} BC &= D \Leftrightarrow \\
\text{vec}(AB \mathbb{1}^T) - \text{vec}(\mathbb{1} BC) &= \text{vec}(D) \Leftrightarrow \\
(A \otimes \mathbb{1} - \mathbb{1} \otimes C^T) \text{vec}(B) &= \text{vec}(D) \Leftrightarrow \\
\text{vec}(B) &= (A \otimes \mathbb{1} - \mathbb{1} \otimes C^T)^{-1} \text{vec}(D) \Leftrightarrow \\
B &= \text{mat}[(A \otimes \mathbb{1} - \mathbb{1} \otimes C^T)^{-1} \text{vec}(D)].
\end{aligned}$$

Letting

$$\begin{aligned} A &= H_j^{(0)}, \\ B &= S_{j,k}^{(m)}, \\ C &= H_k^{(0)}, \\ D &= -iH_{x_{j,k}}^{(m)}, \end{aligned}$$

allows for $S_{j,k}^{(m)}$ to be solved at each order m .

c. Summary of results for perturbative construction

The main result is

$$H_{\text{eff}} = U^\dagger H U = \sum_{m=0}^{\infty} \lambda^m H^{(m)},$$

where

$$\begin{aligned} H^{(m)} &= H^{(m)}(\{S_j\}_{j=1}^m, H_0, H_1) \\ &= i[S_m, H_0] + H_x^{(m)}(\{S_j\}_{j=1}^{m-1}, H_0, H_1). \end{aligned}$$

At each order m , $H_x^{(m)}$ is a function of only $\{S_1, \dots, S_{m-1}\}$ and so can be computed since we assume the lower order $\{S_1, \dots, S_{m-1}\}$ is known. Hence, $H^{(m)}(\{S_j\}_{j=1}^m, H_0, H_1)$ has only one term containing S_m , $i[S_m, H_0]$. Solving for S_m subject to the desired dynamics allows for computation of $H^{(m)}$. For instance, in the case of the SW transformation, the desired dynamics is to have $H^{(m)}$ be block diagonal on H_l and H_e .

We have

$$\begin{aligned} H^{(0)} &= H_0, \\ H_x^{(1)} &= H_1. \end{aligned}$$

If $H^{(m)}$ is block diagonal,

$$H^{(m)} = H_1^{(m)} \oplus \dots \oplus H_k^{(m)} \oplus \dots,$$

then, since S can without loss of generality be an off-block-diagonal matrix (the block-diagonal entries of S are 0),

$$\begin{aligned} H_j^{(m)} &= H_{x_{j,j}}^{(m)} \text{ if } j = k, \\ H_j^{(0)} S_{j,k}^{(m)} - S_{j,k}^{(m)} H_k^{(0)} &= -iH_{x_{j,k}}^{(m)} \text{ if } j \neq k. \end{aligned}$$

Note that if $H^{(0)}$ is diagonal, then

$$\langle p | S_{j,k}^{(m)} | q \rangle = \frac{-i \langle p | H_{x_{j,k}}^{(m)} | q \rangle}{\langle p | H_j^{(0)} | p \rangle - \langle q | H_k^{(0)} | q \rangle}.$$

If $H^{(0)}$ is not diagonal, we use the following matrix-vector correspondence:

$$(A \otimes B) \text{vec}(C) = \text{vec}(ACB^T),$$

which holds for any A, B, C , where “vec” is defined as $\text{vec}(|a\rangle\langle b|) = |a\rangle \otimes |b\rangle$. Hence,

$$AB - BC = D \Leftrightarrow B = \text{mat}[(A \otimes \mathbb{1} - \mathbb{1} \otimes C^T)^{-1} \text{vec}(D)].$$

Letting $A = H_j^{(0)}$, $B = S_{j,k}^{(m)}$, $C = H_k^{(0)}$, and $D = -iH_{x_{j,k}}^{(m)}$ allows us to solve for $S_{j,k}^{(m)}$ at each order m .

APPENDIX B: MAKING THE RWA IN THE DUFFING MODEL CASE

We move into a frame rotating at ω_d on both qubits. The unitary operator R corresponding to this frame transformation is defined by the Hamiltonian $\tilde{H}_A = \omega_d(b_1^\dagger b_1 + b_2^\dagger b_2)$,

$$R = e^{-i[\omega_d(b_1^\dagger b_1 + b_2^\dagger b_2)]t}.$$

This gives the Hamiltonian

$$\tilde{H}_{\text{sys}}^{(0)} - \tilde{H}_A + R^\dagger \tilde{H}_d R =: \tilde{H}_{\text{drift}} + R^\dagger \tilde{H}_d R.$$

Let us now focus on the term $R^\dagger \tilde{H}_d R$ and make the RWA, which amounts to ignoring all excitations of energy cost $2\omega_d$ or higher.

We have

$$\begin{aligned} R^\dagger \tilde{H}_d R &= \sum_{j=1}^2 [\Omega_{X_j}(t) \cos(\omega_d t) + \Omega_{Y_j}(t) \sin(\omega_d t)] R^\dagger \tilde{B}_j R \\ &= \sum_{j=1}^2 \left[\Omega_{X_j}(t) \left(\frac{e^{i\omega_d t} + e^{-i\omega_d t}}{2} \right) \right. \\ &\quad \left. - i\Omega_{Y_j}(t) \left(\frac{e^{i\omega_d t} - e^{-i\omega_d t}}{2} \right) \right] R^\dagger \tilde{B}_j R. \end{aligned}$$

First, let us analyze the term $R^\dagger \tilde{B}_1 R$,

$$R^\dagger \tilde{B}_1 R = e^{-i\omega_d(b_1^\dagger b_1 + b_2^\dagger b_2)t} \tilde{B}_1 e^{i\omega_d(b_1^\dagger b_1 + b_2^\dagger b_2)t}.$$

Let

$$\tilde{B}_1 = \sum_{i_1, i_2, j_1, j_2} \tilde{B}_1^{i_1, i_2, j_1, j_2} |i_1 d + i_2\rangle \langle j_1 d + j_2|$$

and

$$e^{-i\omega_d(b_1^\dagger b_1 + b_2^\dagger b_2)t} = \sum_{i_1, i_2} e^{-i\omega_d t(i_1 + i_2)} |i_1 d + i_2\rangle \langle i_1 d + i_2|,$$

where the index in each sum is taken from 0 to $d-1$. If $\vec{i} = (i_1, i_2)$, $\vec{j} = (j_1, j_2)$, then

$$R^\dagger \tilde{B}_1 R = \sum_{\vec{i}, \vec{j}} e^{-i\omega_d t(i_1 + i_2 - j_1 - j_2)} \tilde{B}_1^{\vec{i}, \vec{j}} |i_1 d + i_2\rangle \langle j_1 d + j_2|,$$

and so, if

$$\Omega_j := \Omega_{X_j}(t) \left(\frac{e^{i\omega_d t} + e^{-i\omega_d t}}{2} \right) - i\Omega_{Y_j}(t) \left(\frac{e^{i\omega_d t} - e^{-i\omega_d t}}{2} \right),$$

then

$$\begin{aligned} R^\dagger \tilde{H}_d R &= \Omega_1 \sum_{\vec{i}, \vec{j}} e^{-i\omega_d t(i_1 + i_2 - j_1 - j_2)} \tilde{B}_1^{\vec{i}, \vec{j}} |i_1 d + i_2\rangle \langle j_1 d + j_2| \\ &\quad + \Omega_2 \sum_{\vec{i}, \vec{j}} e^{-i\omega_d t(i_1 + i_2 - j_1 - j_2)} \tilde{B}_2^{\vec{i}, \vec{j}} |i_1 d + i_2\rangle \langle j_1 d + j_2|. \end{aligned}$$

Now we want to ignore all terms rotating at $2\omega_2$ or higher. Let us focus on the $\Omega_{X_1}(t)$ term first. We have

$$\begin{aligned} \Omega_{X_1}(t) & \frac{e^{i\omega_1 t} + e^{-i\omega_1 t}}{2} e^{-i\omega_1 t(i_1+i_2-j_1-j_2)} \tilde{B}_1^{\vec{i},\vec{j}} \\ & = \frac{\Omega_{X_1}(t)}{2} \tilde{B}_1^{\vec{i},\vec{j}} [e^{i\omega_1 t(1-i_1-i_2+j_1+j_2)} + e^{-i\omega_1 t(1+i_1+i_2-j_1-j_2)}], \\ -i\Omega_{Y_1}(t) & \frac{e^{i\omega_1 t} + e^{-i\omega_1 t}}{2} e^{-i\omega_1 t(i_1+i_2-j_1-j_2)} \tilde{B}_1^{\vec{i},\vec{j}} \\ & = \frac{-i\Omega_{Y_1}(t)}{2} \tilde{B}_1^{\vec{i},\vec{j}} [e^{i\omega_1 t(1-i_1-i_2+j_1+j_2)} - e^{-i\omega_1 t(1+i_1+i_2-j_1-j_2)}], \\ \Omega_{X_2}(t) & \frac{e^{i\omega_2 t} + e^{-i\omega_2 t}}{2} e^{-i\omega_2 t(i_1+i_2-j_1-j_2)} \tilde{B}_2^{\vec{i},\vec{j}} \\ & = \frac{\Omega_{X_2}(t)}{2} \tilde{B}_2^{\vec{i},\vec{j}} [e^{i\omega_2 t(1-i_1-i_2+j_1+j_2)} + e^{-i\omega_2 t(1+i_1+i_2-j_1-j_2)}], \\ -i\Omega_{Y_2}(t) & \frac{e^{i\omega_2 t} + e^{-i\omega_2 t}}{2} e^{-i\omega_2 t(i_1+i_2-j_1-j_2)} \tilde{B}_2^{\vec{i},\vec{j}} \\ & = \frac{-i\Omega_{Y_2}(t)}{2} \tilde{B}_2^{\vec{i},\vec{j}} [e^{i\omega_2 t(1-i_1-i_2+j_1+j_2)} - e^{-i\omega_2 t(1+i_1+i_2-j_1-j_2)}]. \end{aligned}$$

Looking at the terms in the brackets on the right-hand side, we see that

$$\left\{ \begin{array}{l} \text{if } |i_1 + i_2 - j_1 - j_2| \neq 1, \text{ then} \\ e^{i\omega_1 t(1-i_1-i_2+j_1+j_2)} = 0, \quad e^{-i\omega_1 t(1+i_1+i_2-j_1-j_2)} = 0; \\ \text{if } i_1 + i_2 - j_1 - j_2 = 1, \text{ then} \\ e^{i\omega_1 t(1-i_1-i_2+j_1+j_2)} = 1, \quad e^{-i\omega_1 t(1+i_1+i_2-j_1-j_2)} = 0; \\ \text{if } i_1 + i_2 - j_1 - j_2 = -1, \text{ then} \\ e^{i\omega_1 t(1-i_1-i_2+j_1+j_2)} = 0, \quad e^{-i\omega_1 t(1+i_1+i_2-j_1-j_2)} = 1. \end{array} \right.$$

Hence, in total,

$$\left\{ \begin{array}{l} \text{if } |i_1 + i_2 - j_1 - j_2| \neq 1, \text{ then } (RH_{d,\text{diag}}R^\dagger)_{i_1,i_2,j_1,j_2} = 0; \\ \text{if } i_1 + i_2 - j_1 - j_2 = 1, \text{ then} \\ (R\tilde{H}_dR^\dagger)_{i_1,i_2,j_1,j_2} = \frac{\Omega_{X_1}(t)-i\Omega_{Y_1}(t)}{2} \tilde{B}_1^{\vec{i},\vec{j}} \\ \quad + \frac{\Omega_{X_2}(t)-i\Omega_{Y_2}(t)}{2} \tilde{B}_2^{\vec{i},\vec{j}}; \\ \text{if } i_1 + i_2 - j_1 - j_2 = -1, \text{ then} \\ (R\tilde{H}_dR^\dagger)_{i_1,i_2,j_1,j_2} = \frac{\Omega_{X_1}(t)+i\Omega_{Y_1}(t)}{2} \tilde{B}_1^{\vec{i},\vec{j}} \\ \quad + \frac{\Omega_{X_2}(t)+i\Omega_{Y_2}(t)}{2} \tilde{B}_2^{\vec{i},\vec{j}}. \end{array} \right.$$

The full rotating-wave-approximated Hamiltonian becomes

$$H_{\text{RWA}} = \tilde{H}_{\text{drift}} + \tilde{H}_{d,\text{RWA}},$$

where

$$\begin{aligned} \tilde{H}_{\text{drift}} & := \tilde{H}_{\text{sys}}^{(0)} - \tilde{H}_A, \\ \tilde{H}_{d,\text{RWA}} & := (R^\dagger \tilde{H}_d R)^{\text{RWA}}, \\ \tilde{H}_A & = \omega_d(b_1^\dagger b_1 + b_2^\dagger b_2), \end{aligned} \quad (\text{B1})$$

and the matrix elements of $(R^\dagger H_{d,\text{diag}} R)^{\text{RWA}}$ are as defined by the above cases.

APPENDIX C: PAULI COEFFICIENTS

The full set of Pauli coefficients of the form $A \otimes B$ for $A \in \{I, Z\}$ and $B \in \{I, X, Y, Z\}$ are given below,

$$\begin{aligned} \frac{IX}{2 \text{ coeff}} & = -\frac{J\Omega}{\Delta + \delta_1} + \frac{\Delta \delta_1 J\Omega^3}{(\Delta + \delta_1)^3(2\Delta + \delta_1)(2\Delta + 3\delta_1)}, \\ \frac{IY}{2 \text{ coeff}} & = 0, \\ \frac{IZ}{2 \text{ coeff}} & = \frac{J^2\Omega^2}{2} \left[\frac{\delta_1^3 - 2\delta_1\Delta^2 - 2\Delta^3}{\delta_1\Delta^2(\delta_1 + \Delta)^2(\Delta - \delta_2)} + \frac{\delta_1^2 + \Delta^2}{\Delta^2\delta_2(\delta_1 + \Delta)^2} \right. \\ & \quad + \frac{6\delta_1^5 + 4\delta_1^4\Delta - 6\delta_1^3\Delta^2 + 7\delta_1^2\Delta^3 + 12\delta_1\Delta^4 + 4\Delta^5}{\Delta^2(\delta_1 + \Delta)^2(2\delta_1 + \Delta)^2(\delta_1 + 2\Delta)(3\delta_1 + 2\Delta)} \\ & \quad + \frac{2}{\delta_1(\delta_1 + \Delta)(\delta_1 + \Delta - \delta_2)} \\ & \quad \left. + \frac{2}{(\delta_1 + \Delta)(\delta_1 + \Delta - \delta_2)^2} + \frac{1}{\Delta(\Delta - \delta_2)^2} \right], \\ \frac{ZI}{2 \text{ coeff}} & = -\frac{\delta_1\Omega^2}{2\Delta(\delta_1 + \Delta)} \\ & \quad + \frac{J^2\Omega^2}{2(\delta_1 + \Delta)^3} \left[\frac{2(\delta_1^2 + \delta_1\Delta + \Delta^2)(\delta_1 + \Delta)}{\delta_1\Delta(\delta_2 - \Delta)} \right. \\ & \quad + \frac{1}{2}\delta_1 \left(\frac{4\delta_1^2}{\Delta^3} + \frac{11\delta_1}{\Delta^2} + \frac{3\delta_1}{(2\delta_1 + \Delta)^2} \right. \\ & \quad \left. \left. - \frac{2}{\delta_1 + 2\Delta} - \frac{6}{3\delta_1 + 2\Delta} + \frac{12}{\Delta} \right) \right. \\ & \quad + \frac{2(\delta_1 + \Delta)^2}{\delta_1(\delta_1 + \Delta - \delta_2)} + \frac{2(\delta_1 + \Delta)^2}{(\delta_1 + \Delta - \delta_2)^2} \\ & \quad \left. - \frac{2\delta_1(\delta_1 + \Delta)}{\Delta\delta_2} \right], \\ \frac{ZX}{2 \text{ coeff}} & = -\frac{J\Omega}{\Delta} \left(\frac{\delta_1}{\delta_1 + \Delta} \right) \\ & \quad + \frac{J\Omega^3\delta_1^2(3\delta_1^3 + 11\delta_1^2\Delta + 15\delta_1\Delta^2 + 9\Delta^3)}{2\Delta^3(\delta_1 + \Delta)^3(\delta_1 + 2\Delta)(3\delta_1 + 2\Delta)}, \\ \frac{ZY}{2 \text{ coeff}} & = 0, \\ \frac{ZZ}{2 \text{ coeff}} & = \frac{J^2}{2(\delta_1 + \Delta)^2} \left(\Omega^2 \left\{ \frac{\delta_1^3 - 2\delta_1\Delta^2 - 2\Delta^3}{\delta_1\Delta^2(\delta_2 - \Delta)} \right. \right. \\ & \quad + \frac{1}{2} \left[\frac{4(3\delta_1 + \Delta)(\delta_1^2 + \delta_1\Delta + \Delta^2)}{\Delta^2(2\delta_1 + \Delta)^2} \right. \\ & \quad \left. \left. - \frac{16\Delta}{3\delta_1^2 + 8\delta_1\Delta + 4\Delta^2} \right] \right. \\ & \quad \left. + \frac{2\delta_1}{\Delta\delta_2} - \frac{2(\delta_1 + \Delta)}{(\delta_1 + \Delta - \delta_2)^2} - \frac{2(\delta_1 + \Delta)}{\delta_1(\delta_1 + \Delta - \delta_2)} \right) \\ & \quad + \frac{2(\delta_1 + \Delta)(\delta_1 + \delta_2)}{\Delta - \delta_2} \Big). \end{aligned}$$

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